



Certificate of Analysis

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Product Name: Teriflunomide Catalog No.: 5069 Batch No.: 2

CAS Number: 108605-62-5

IUPAC Name: 2-Cyano-3-hydroxy-*N*-[4-(trifluoromethyl)phenyl]-2-butenamide

1. PHYSICAL AND CHEMICAL PROPERTIES

Batch Molecular Formula: $C_{12}H_9F_3N_2O_2$.

Batch Molecular Weight: 270.21

Physical Appearance: White solid

Solubility: DMSO to 100 mM Storage: Store at +4°C

Batch Molecular Structure:

2. ANALYTICAL DATA

HPLC: Shows 99.6% purity

¹H NMR: Consistent with structure

Mass Spectrum: Consistent with structure

Microanalysis: Carbon Hydrogen Nitrogen

Theoretical 53.34 3.36 10.37 Found 53.42 3.32 10.35



Product Information

Print Date: Mar 16th 2022

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IUPAC Name: 2-Cyano-3-hydroxy-*N*-[4-(trifluoromethyl)phenyl]-2-butenamide

Description:

Teriflunomide is an inhibitor of dihydroorotate dehydrogenase (K_d = 12 nM; K_i = 179 nM). Inhibits proliferation of mitogen- or cytokine-stimulated lymphoid cells in vitro by inhibiting cell cycle progression from G_1 to S. Immunosuppressive agent. Active metabolite of leflunomide.

Physical and Chemical Properties:

Batch Molecular Formula: $C_{12}H_9F_3N_2O_2$.

Batch Molecular Weight: 270.21 Physical Appearance: White solid

Minimum Purity: ≥99%

Batch Molecular Structure:

Storage: Store at +4°C

Solubility & Usage Info:

DMSO to 100 mM

Stability and Solubility Advice:

Some solutions can be difficult to obtain and can be encouraged by rapid stirring, sonication or gentle warming (in a 45-60°C water bath).

Information concerning product stability, particularly in solution, has rarely been reported and in most cases we can only offer a general guide. Our standard recommendations are:

SOLIDS: Provided storage is as stated on the product label and the vial is kept tightly sealed, the product can be stored for up to 6 months from date of receipt.

SOLUTIONS: We recommend that stock solutions, once prepared, are stored aliquoted in tightly sealed vials at -20°C or below and used within 1 month. Wherever possible solutions should be made up and used on the same day.

References:

Iglesias-Bregna *et al* (2013) Effects of prophylactic and therapeutic teriflunomide in transcranial magnetic stimulation-induced motor-evoked potentials in the dark agouti rat model of experimental autoimmune encephalomyelitis. J.Pharmacol.Exp.Ther. **347** 203. PMID: 23892570

Davis *et al* (1996) The immunosuppressive metabolite of leflun. is a potent inhibitor of human dihydroorotate dehydrogenase. Biochemistry **35** 1270. PMID: 8573583.

Williamson et al (1995) Dihydroorotate dehydrogenase is a high affinity binding protein for A77 1726 and mediator of a range of biological effects of the immunomodulatory compound. J.Biol.Chem. 270 22467. PMID: 7673235.

Caution - Not Fully Tested • Research Use Only • Not For Human or Veterinary Use